Intergovernmental Oceanographic
Commission of UNESCO

World
Meteorological Organization

DATA BUOY COOPERATION PANEL

SEA SURFACE SALINITY QUALITY CONTROL PROCESSES FOR POTENTIAL USE ON DATA BUOY OBSERVATIONS

DBCP Technical Document No. 42

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D A T A B U O Y C O O P E R A T I O N P A N E L

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DOCUMENT REVISION HISTORY

Date	Modification	Who	Version
October 2010	First draft reviewed by DBCP-26	Hester Viola	1.0
25 May 2011	Editorial changes Updated information on user requirements Added list of acronyms	WMO Secretariat	1.1
July 2011	Review by DBCP Task Teams on Instrument Best Practices and Drifter Technology Development (TT-IBP), and Data Management (TT-DM)	TT-IBP, TT-DM	1.2
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SEA SURFACE SALINITY QUALITY CONTROL PROCESSES FOR POTENTIAL USE ON DATA BUOY OBSERVATIONS

1 Background

At the 26th session of the Data Buoy Cooperation Panel (DBCP) in 2009, the Panel recognised that there was a need for the development of quality control processes for Sea Surface Salinity measurements as more buoys would be measuring this important parameter in the near future, initially as ground truthing for Satellite Calibration and then ongoing for Satellite validation.

It must be noted that the major challenge in measuring Sea Surface Salinity (SSS) is stability over time and resistance to fouling, which is of particular concern for drifting buoys. The cost of the SSS sensor versus the cost of the whole buoys is also an important consideration. To provide ground truthing of satellites such as SMOS[1]/Aquarius[2] the accuracy does not need to be very high so a relatively inexpensive sensor should be viable.

Many panel members suggested that they could provide documents or tools for assessing Quality Control (QC) for SSS. It was agreed that the Panel members provide details of Sea Surface Salinity quality control processes to the Joint WMO-IOC Technical Commission for Oceanography and Marine Meteorology (JCOMM) *in situ* Observations Programme Support Centre (JCOMMOPS) for compilation into a best practice document for review by the community.

2 Aim

This document will aim to provide processes and approaches to real-time and delayed mode quality control of Sea Surface Salinity data, for review by the DBCP community. This document aims to bring together the best practice and suggested approaches to quality controlling salinity data from various programmes and for several different types of observing platforms. Once the DBCP has ascertained which processes apply to drifting and moored buoys, the appropriate tests and procedures can be added to DBCP Technical documents which already exist.

3 Other related documents

For general data processing information and quality control processes to apply to all data being shared on the WMO's World Weather Watch (WWW) Global Telecommunication System (GTS), refer to DBCP Technical Document 2 or 37 available via the WMO website: http://www.wmo.int/pages/prog/amp/mmop/dbcp_reports.html

Other documentation relating to the Data Buoy Cooperation Panel are referenced here: http://www.jcommops.org/dbcp/community/standards.html

1 SMOS: European Space Agency's Soil Moisture and Ocean Salinity satellite mission - http://www.esa.int/esaLP/LPsmos.html

2 Aquarius satellite mission for measuring Sea Surface Salinity, developped jointly by the US National Aeronautics and Space Administration (NASA) and the Space Agency of Argentina (Comisión Nacional de Actividades Espaciales) - http://aquarius.nasa.gov/

4 Inputs to this Document

Advice was provided by the following groups:

- Global Drifter Center (initial approaches to QC and question to IFREMER[3])
- Météo-France (Model comparisons to Mercator[4] model)
- IFREMER/Europe (techniques applied to SMOS/Aquarius Calibration and Validation)

Documents used:

- DBCP Technical Documents 3 - Guide to Data Collection and Location Services using Service Argos
- DBCP Technical Document No. 37 - Guide to buoy data quality control tests to perform in real-time by a GTS data processing centre
- Argo[5] manual (for QC of salinity/temperature profiles)
- Global Temperature and Salinity Programme (GTSPP) (for QC flags) website[6] and manuals
- Global Ocean Surface Underway Data (GOSUD) quality control procedures (especially those documented by the Atlantic Oceanographic and Meteorological Laboratory (AOML) for thermosalinograph observations)
- Carbon-Ops documents[7] by the British Oceanographic Data Centre (BODC)
- Quality Assurance of Real Time Oceanographic Data (QARTOD[8]) (Real time QC recommendations) – though at this point processes for quality controlling salinity are not explicitly covered.

3 IFREMER : French Research Institute for Exploration of the Sea - http://www.ifremer.fr
4 http://www.mercator-ocean.fr/
5 http://www.argo.net
6 http://www.nodc.noaa.gov/GTSPP/
7 http://www.bodc.ac.uk/carbon-ops/data/processing/
8 http://qartod.org

5 Requirements for SSS measurement (Accuracy, timings & resolutions)

The Ocean Observations Panel for Climate (OOPC[9]), and its predecessors examined the usefulness of surface salinity data in the context of climate change detection. They state that "At high latitude, sea surface salinity is known to be critical for decadal and longer time scale variations associated with deep ocean over turning and the hydrological cycle. In the tropics, and in particular in the western Pacific, and Indonesian Seas, and in upwelling zones, salinity is also believed to be important." They quote the benchmark sampling strategy to be one sample per 200 km square every 10 days and with an accuracy of 0.1 PSU. They also state that the tropical western Pacific and Indian Oceans and high latitudes should receive the highest priority.

Table 1 below provides for the requirements for Ocean Salinity measurements as documented in the WMO Rolling review of Requirements (RRR) Database[10] for the atmospheric (AOPC[11]) and ocean (OOPC) domains of the Global Climate Observing Systems (GCOS), as well as for Global Numerical Weather Prediction. Each requirement is expressed in terms of Horizontal Resolution, Vertical Resolution, Observing Cycle, Delay of Availability and Accuracy (psu – practical salinity unit) with each parameter described in terms of Goal, Breakthrough (B/T) and Threshold (T/H).

Layer	Application	Source	Accuracy Goal/Bk/Threshold			Horizontal Resolution Goal/Bk/Threshold			Vertical Resolution Goal/Bk/Threshold			Observing Cycle Goal/Bk/Threshold			Delay of availability Goal/Bk/Threshold		
Sea surface	Global NWP	WMO	0.1 psu	0.2 psu	0.3 psu	5 km	100 km	250 km				1 d	30 d	60 d	3 h	24 h	120 h
Sea surface	Seasonal to inter-annual climate prediction	WMO	0.1 psu	0.144 psu	0.3 psu	100 km	135.7 km	250 km				30 d	40 d	60 d	9 d	21.3 d	120 d
Sea surface	CLIVAR	WCRP	0.1 psu	0.144 psu	0.3 psu	100 km	135.7 km	250 km				30 d	37.8 d	60 d	9 d	21.3 d	120 d
Sea surface	GOOS Climate - large scale	GOOS	0.1 psu	0.215 psu	1 psu	200 km	271.4 km	500 km				10 d	14.4 d	30 d	10 d	14.4 d	30 d
Sea surface	OOPC	GCOS	0.05 psu	0.09 psu	0.3 psu	100 km	170 km	500 km				7 d	11 d	30 d	10 d	15 d	30 d
Upper ocean	OOPC	GCOS	0.001 psu	0.002 psu	0.01 psu	15 km	40 km	300 km	1 m	2 m	10 m	1 d	2 d	10 d	0.5 h	0.6 h	1 h
Upper ocean	Global NWP	WMO	0.1 psu	0.2 psu	0.3 psu	5 km	100 km	250 km	1 m	2 m	10 m	1 d	30 d	60 d	3 h	24 h	120 h
Deep ocean	OOPC	GCOS	0.002 psu	0.003 psu	0.005	50 km	60 km	100 km	2 m	2.5 m	4 m	30 d	70 d	360 d	60 d	110 d	360 d

Table 1: Observational Requirements for Salinity (from the WMO Rolling review of Requirements Database)

9 http://ioc-goos-oopc.org/

10 http://www.wmo.int/pages/prog/sat/Databases.html

11 Atmospheric Observation Panel for Climate - http://www.wmo.int/pages/prog/gcos/index.php?name=AOPC

6 Suggested Quality Control processes

6.1 Computation of salinity based upon conductivity, temperature, and depth

Salinity is required to measure the presence and movement of water masses in the ocean. Salinity is a derived product and some instruments provide the salinity directly (through internal calculations) and others provide the conductivity, temperature, and depth required to calculate the salinity. Salinity measurements have been made at a number of coastal stations and recently at a number of coastal buoys. Several different instruments have been used to measure the salinity. Usually salinity measurements are based on the practical salinity scale using the empirical relationship between the salinity and conductivity of seawater. The salinity units are reported in practical salinity units (psu).

The calculation of salinity is based on conductivity and the concomitant temperature measurement in the platform. If either measurement is missing or flagged suspect by the automated quality control then salinity is not derived. (http://www.bodc.ac.uk/carbon-ops/data/processing/#nrt_proc)

Where salinity is computed based upon water conductivity (C), temperature (T), and depth (D) values the computation should follow platform operator specifications.

Alternatively, to compute salinity prior to use or distribution the following documents give advice:

- EOS-80 “Practical Salinity Scale 1978 and International Equation of State of Seawater 1980” and uses computed values of C, T, and D,.
- In June 2009 experts attending the 25th Assembly of UNESCO's Intergovernmental Oceanographic Commission (IOC) in Paris recommended through Resolution 7 to adopt the International Thermodynamic Equation of Seawater (TEOS-10) formulation that has been developed and recommended by the International Association for the Physical Sciences of the Oceans (IAPSO) Scientific Committee on Oceanic Research (SCOR) WG-127[12] to replace the existing EOS-80, as presented in the TEOS-10 Manual (see Annex I for references).

There are processes documented for sub-surface salinity for the Argo program and GTSPP, though they mostly rely on the adjacent values in the profile, which may not be present for a drifter.

The GOSUD program also suggests a process of 10 different real time quality control tests to perform. All the Thermosalinograph (TSG) data received by AOML in real-time undergo a series of QC tests to ensure that only data of good quality are stored and distributed. The most important QC steps in the GOSUD real-time procedure are checks on: Date, Location, Global sea surface salinity and temperature ranges, Regional sea surface salinity and temperature ranges, Detection of spikes along the track, Gradient, Constant value and Climatology.

Apart from the test on Date and Time, which are assumed to be independent of the salinity measurement itself and are at an observation level, these tests are explained further.

12: http://www.scor-int.org/Working_Groups/wg127.htm

6.2 Tropical Atmosphere Ocean (TAO) array

Salinity values are calculated from measured conductivity and temperature data using the method of Fofonoff and Millard (1983). Surface salinity records are plotted and examined for periods of spiky data caused by response time differences between conductivity and temperature sensors. The identified spiky periods are flagged. If necessary, conductivity values from all depths are adjusted for sensor calibration drift by linearly interpolating over time between values calculated from the pre-deployment calibration coefficients and those derived from the post-deployment calibration coefficients.

A thirteen point Hanning filter is applied to the high-resolution (ten minute interval) conductivity and temperature data. A filtered value is calculated at any point for which seven of the thirteen input points are available. The missing points are handled by dropping their weights from the calculation, rather than by adjusting the length of the filter. Salinity values are recalculated from the filtered data and subsampled to hourly intervals.

Delayed mode daily salinity and density values are calculated by taking the mean of the available hourly values for the day. If there are fewer than 12 hourly values available, a daily mean value is not computed.

http://tao.noaa.gov/proj_overview/qc_ndbc.shtml

6.3 National Data Buoy Center Quality Control of Salinity from Moored Buoys

Salinity (ZSAL1) is calculated from the conductivity (ZCOND1) and temperature (ZTMP1) collected by the SeaBird 39-SM or the Falmouth Scientific Instruments (FSI) unit.

> **PASS -2° C ≤ ZTMP1 ≤ 40° C (Water temperature EQC limits are often substituted)**
>
> **PASS 0 ≤ ZCOND1 ≤ 7 Siemens/m**
>
> **PASS 0 ≤ ZSAL1 ≤ 42 psu. (Station specific limits are often substituted)**

Salinity is also provided by the Ocean Sensor Module (OSM), a derivative of the SeaKeepers 1000. Salinity is provided directly from the OSM unit.

> **PASS -2° C ≤ ZSTMP1 ≤ 40° C (Water temperature EQC limits are often substituted)**
>
> **PASS 0 ≤ ZSCOND ≤7 Siemens/m**
>
> **PASS 0 ≤ ZSSAL ≤ 42 psu Station specific limits are often substituted)**

http://www.ndbc.noaa.gov/NDBCHandbookofAutomatedDataQualityControl2009.pdf

6.4 IFREMER/LOCEAN

IFREMER/LOCEAN provided a procedure which it has developed, on behalf of the European programmes, quality control processing for SSS drifters deployed over the last five years in preparation for SMOS (and now for the SMOS satellite cal-val phase).

As of 2010, the approach includes four steps: carried out for the most part in delayed mode (but could be applied in real time, aside from the challenges of automating the approach, and potential human resource issues.)

1. identifying isolated spikes that might be related to mis-transmission of data or erroneous data acquisition.(a tricky step, to mitigate the removal of rainfall; which seems easier to do when data are acquired every half hour (or higher frequency) than when data are hourly);
2. removing (flag as bad) portions of records obviously erroneous (as a result of heavy fouling, or when an object is temporarily stuck in the conductivity cell); this is detected by identifying sudden negative jumps in S (larger than -0.1) with no associated variation in T (less than 0.05), and are not rainfall induced. This cannot reliably be done in real-time or at least before having one day elapsed;
3. removing (flagging) artificial day-time variations when Sea Surface Temperature (SST) daily cycle is large (due to difference between depth of conductivity cell/depth of temperature measurement);
4. correcting drifts (light fouling, corrosion, deposits, electronics...) is usually done by linear fit, in salinity based on collocating salinity drifters with nearby Argo floats (or other 'reliable' comparisons that might be available).

This is work in progress, and so far these tests have been undertaken for different generations of drifters manufactured since 2005 by Pacific Gyre and Metocean, and for home-made drifters/floats at LOCEAN (Paris) and ICM/CSIC (Barcelona); the results will be fully reported in 2011.

http://www.locean-ipsl.upmc.fr/smos/drifters

6.5 Global Temperature - Salinity Profile Program (GTSPP)

The GTSPP suggests quality control tests and flags to use on data
http://www.nodc.noaa.gov/GTSPP/document/qcmans/GTSPP_RT_QC_Manual_20090916.pdf

Tests such as the impossible value (gross error) or freezing point test, spike and gradient tests are all included in the document. Data quality flags are described here: http://www.nodc.noaa.gov/GTSPP/document/qcmans/qcflags.htm

6.6 Global Ocean Surface Underway Data Pilot Project (GOSUD)

The GOSUD process includes real-time test and could also be used in delayed mode, with a few additions.

For example, at AOML, for Quality control procedures in delayed-time mode, several additional QC steps are conducted in delayed-mode. As described in its QC procedures sheet: http://www.aoml.noaa.gov/phod/tsg/data/qc_sheet.pdf which may be useful/adaptable for buoys as well . The delayed mode component of this procedure includes the following tests –

Step 11: Climatology and NCEP weekly analysis	Each measurement is compared against a monthly climatology (Levitus 2001, 1°x1°, monthly) and against the US National Center for Environmental Prediction (NCEP) weekly analysis fields.
Step 12: Buddy check	Each measurement is compared with profiling floats, Expendable Bathythermographs (XBTs), CTDs, thermistor chain and drifter data (referred here as 'buddy') within 100 km and ± 5 days of the TSG measurement. The value to be checked is subtracted from the value of the buddy. • Temperature: The value is flagged when the difference exceeds 0.5°C • Salinity: The value is flagged when the difference exceeds 0.2psu Note that Buddy data will not always be available.
Step 13: Water Samples	Salinity data are compared against salinity measurements derived from water samples taken during the transect (if available).
Step 14: Calibrations	Data are corrected using the calibration coefficients provided by the manufacturer.

Table 3: Additional Delayed mode test performed by AOML on TSG data

On doubtful data a visual check by ocean physics experts is performed and the responsible DAC is warned in case an anomaly is detected.

7 Gross Error or Broad Range Check

For each kind of geophysical variable, sensor data should be compared with constant limits. Out-of-range data are not sent onto the GTS. Note that limit values are considered as valid. This table is based on the "Operational Measurement Uncertainty Requirements and Instrument Performance" listed in WMO-8 Guide to Meteorological Instruments and Methods of Observation.

Parameter	Lower limit	Upper limit
Sea level air pressure (hPa)	500	1080
Water temperature (deg C)	- 7	+ 45
Air temperature (deg)	- 40	+ 50
Wind speed (m/s)	0	62
Wind direction (deg)	0	360
Salinity (psu)	10	70

Table 2: Recommended gross error checks for typical marine variables

GTSPP suggests that between 0 and 41 psu are realistic values for depth of 0-25m and GOSUD suggests 0.0 to 60 PSU.

Regional ranges are given for the Mediterranean and Red Seas, so these areas could be treated differently in real time tests, though this is less necessary for salinity than for Temperature.

7.1 User defined limit check (or climatological test)

Each sensor measurement is compared with limits provided by the platform operator based on climatological data for the area where the platform is expected to be reporting from. Each sensor can have its own limits. Out-of-range data should be flagged and/or suppressed. Note that limit values are considered as valid.

Alternatively, the limits could be automatically extracted from a climatological file based upon a query at the actual position of the platform at the time of reporting. There are various climatologies that could be applied. Checks usually involve testing against 3-5 standard deviations from the norm of the climatology, depending on the bathymetry.

Marine climatology data can be requested from the International Comprehensive Ocean-Atmosphere Data Set (ICOADS). More details on ICOADS and how to access the data on its web site are available at: http://icoads.noaa.gov/products.html.

7.2 Temperature and/or Salinity profile Spike test

Differences between sequential measurements, where one measurement is quite different than adjacent ones, is a spike in both size and gradient.

Test value = | V2 - (V3 + V1)/2 | - | (V3 - V1) / 2 |

where V2 is the measurement being tested as a spike, and V1 and V3 are the values previous and next.

- Temperature: The V2 value is flagged when the test value exceeds 6.0 degree C.
- Salinity: The V2 value is flagged when the test value exceeds 0.9 PSU

Values that fail the spike test should be flagged as wrong and should not be distributed.

This test was initially introduced for the Argo programme. The test should fail if a data point (Depth, Temp. and/or Sal.) value departs too much from nearby points after the profile was ordered by decreasing depth (i.e. towards surface). The test is only applied to WATER TEMPERATURE (PROBE) and WATER SALINITY types of sensors.

In case the temperature sensor values or salinity sensor values alone fail the test, then values from that sensor should not be used in real-time. If they both fail the test then the whole data point (Depth, Temp., Sal.) is rejected. The first and the last data point from the profile do not go through this test. See the Argo quality control manual for further details.

7.3 Temperature and/or Salinity profile Gradient test

This test was initially introduced for the Argo programme. The result is considered bad in the case that the temperature or salinity gradient is too high once the profile is ordered by decreasing values of depth (i.e. towards sea surface). This test is made only for WATER TEMPERATURE (PROBE) and WATER SALINITY types of sensor.

In case the temperature values are rejected then the whole data point (Depth, Temp., Sal.) is rejected. The first and the last data point from the profile will not go through this test. See the Argo quality control manual for details (references in Annex I).

This test is failed when the difference between adjacent measurements is too steep.

Test value = $| V2 - (V3 + V1)/2 |$

where V2 is the measurement being tested as a spike, and V1 and V3 are the previous and next values.

- Temperature: The V2 value is flagged when the test value exceeds 9.0 degree C.
- Salinity: The V2 value is flagged when the test value exceeds 1.5 PSU

Values that fail the test (i.e. value V2) should be flagged as wrong.

7.4 Constant value test

This test was initially introduced for the Argo programme. This test should fail in the case where all values for the same type of sensor are identical along the profile. This test is only applied to WATER TEMPERATURE (PROBE) and WATER SALINITY types of sensor. In case the temperature sensor values are rejected then whole data point (Depth, Temp., Sal.) is rejected. See the Argo quality control manual for details (references in Annex I).

7.5 Checking against surrounding platforms - “Buddy Check”

Regarding SSS QC, Dr Rick Lumpkin from AOML suggested that the first test to implement is a "buddy check" against nearby Argo floats (looking at ~4m depth), Ships (Conductivity-Temperature-Depth measurement (CTDs) or TSG at 1-2 m depth) or Moorings, in addition to the more straightforward check against climatology. Though this does not take into account vertical salinity gradients in the upper 5 m. This test might be difficult to conduct in real-time.

7.6 Visual check of data against Model outputs

Meteo-France has extended its Quality Control tools to produce comparisons between SSS observed by data buoys and co-located Mercator model outputs, for the past two weeks, as done for other parameters. The graphs are updated every day with the data produced the day before. Look at http://www.meteo.shom.fr/qctools/ then click on "Plots of data and differences with model outputs" (grey column). Enter the WMO Id of a salinity buoy on the GTS (e.g. 31739), choose "QC plot" for "Salinity" then "OK". The graph of differences should appear. This can be done in near real time.

8 Delayed mode quality control procedures

Delayed mode processing implies a manual procedure whereby a data expert redoes the above quality control checks, then performs a visual check; undertakes inter-comparisons with other platforms; and cross-checks the data against one or more published climatologies. Their findings and actions will have been fully documented or flagged in the data.

Examples of procedures that the DBCP should consider using in delayed mode are as follows

9 Next steps

This draft document needs to be reviewed and enhanced by the DBCP Task Team on Instrument Best Practices and Drifter Technology Development , the DBCP Task Team on Data Management and DBCP members.

Additions and modifications are sought (send to support@jcommops.org), as required.

References

Fofonoff, P., and R. C. Millard Jr., Algorithms for computation of fundamental properties of seawater, Tech. Pap. Mar. Sci., 44, 53 pp., Unesco, Paris, 1983.

ACRONYMS

AOML	Atlantic Oceanographic and Meteorological Laboratory
AOPC	Atmospheric Observation Panel for Climate (GCOS)
BODC	British Oceanographic Data Centre
CTD	Conductivity-Temperature-Depth measurement
DBCP	Data Buoy Cooperation Panel
ESA	European Space Agency
GCOS	Global Climate Observing System (WMO-IOC-UNEP-ICSU)
GOOS	Global Ocean Observing System (WMO-IOC-UNEP-ICSU)
GOSUD	Global Ocean Surface Underway Data
GTS	Global Telecommunication System
GTSPP	Global Temperature and Salinity Programme
IFREMER	French Research Institute for Exploration of the Sea
IAPSO	International Association for the Physical Sciences of the Oceans
ICOADS	International Comprehensive Ocean-Atmosphere Data Set (USA)
IOC	Intergovernmental Oceanographic Commission of UNESCO
JCOMM	Joint WMO-IOC Technical Commission for Oceanography and Marine Meteorology
JCOMMOPS	JCOMM *in situ* Observations Programme Support Centre
NASA	National Aeronautics and Space Administration
NCEP	NOAA National Center for Environmental Prediction (USA)
NOAA	National Oceanic and Atmospheric Administration (USA)
OOPC	Ocean Observations Panel for Climate
PIRATA	Pilot Research Moored Array in the Tropical Atlantic (TAO)
PSU	Practical Salinity Unit
QARTOD	Quality Assurance of Real Time Oceanographic Data
QC	Quality Control
RAMA	Indian Ocean Research Moored Array for African-Asian-Australian Monsoon Analysis and Prediction (TAO)
RRR	Rolling Review of Requirements (RRR)
SCOR	Scientific Committee on Oceanic Research
SMOS	Soil Moisture and Ocean Salinity (ESA)
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
TAO	Tropical Atmosphere Ocean
TRITON	Triangle Trans-Ocean buoy network (TAO)
TSG	Thermosalinograph
UN	United Nations
UNESCO	UN Educational, Scientific and Cultural Organization
WMO	World Meteorological Organization
WWW	World Weather Watch (WMO)
XBT	Expendable Bathythermograph